AMENDMENTS TO THE SPECIFICATION

Please replace the paragraphs 22, 27, 44, and 53 with the following paragraphs:

[0022] Fig. 11 represents illustrative interaction paths between a water molecule (indicated by arrows) and the fixed structure HIV-1 gp41 protein. The distances is defined between the two atoms on both ends of the arrows except for Fig. 11A ~~Fig. 9A~~ where the distance is defined between the oxygen atom of the water and the center-of-mass of gp41.

[0027] As is well known in the art, there are many different parties providing electronic downloadable information on molecules, such as the ~~. The~~ protein database bank (pdb) ~~at www.pdb.org is an example of one such party~~. The protein database bank website, as well as other sites, are able to provide the molecule as a set of coordinates, with each atom of the molecule having distinct coordinates. A sample set of x, y, and z coordinates obtained from the protein database bank for protein gb41 is provided below:

ATOM	1	N	26.801	20.370	-22.607
ATOM	2	H1	27.720	20.763	-22.465
ATOM	3	H2	26.112	21.023	-22.263
ATOM	4	H3	26.740	20.022	-23.553
ATOM	5	CA	26.672	19.167	-21.736
ATOM	6	HA	25.835	19.339	-21.059
ATOM	7	CB	26.403	17.903	-22.573
ATOM	8	HB	25.490	18.038	-23.152
ATOM	9	CG2	27.574	17.662	-23.520
ATOM	10	1HG2	28.488	17.526	-22.941

[0044] In this calculation, the interaction energy is determined between each of the molecular portions in the first molecule and the second molecule. Interaction energy may be calculated using the well known full quantum mechanical or *ab initio* calculations. However other interaction energy calculations known to those of skill in the art may also be used.

Preferably, software or hardware is used to make the calculations. The Gaussian™ software has the capability of performing full quantum mechanical interaction energies. This program may be obtained at Gaussian's website ~~www.gaussian.com~~. Each of these interaction energies is then added or summed together to provide a total interaction energy of the molecular portions.

[0053] Memory device 130 includes molecule generation module 132 which provides instructions for selecting/generating, i.e., providing, a molecule in the manner described above. For example, molecule generation module 132 can include known electronic downloadable databases, such as the protein database bank~~, located at www.pdb.org~~. Memory 130 also includes molecule decomposing module 134 for accomplishing the decomposing step described above. Molecule decomposing module 134 can also include program code designed to decompose molecules, such as the program code appended to this disclosure. Similarly, cap introduction module 136 includes instructions for accomplishing the cap introduction step described above. This also can be accomplished using the same or different program code designed to decompose the molecule. Finally, energy calculation module 138 includes instructions for calculating the intermolecular interaction energy as described above. The programming steps required for accomplishing energy calculation module 138 are well within the ability of a skilled programmer in light of the functional disclosure provided herein. Energy calculation module 138 can include energy calculation software such as the programs produced by Gaussian™.